U.S. DEPARTMENT OF ENERGY | Office of Science

IMPACT: Benchmarking

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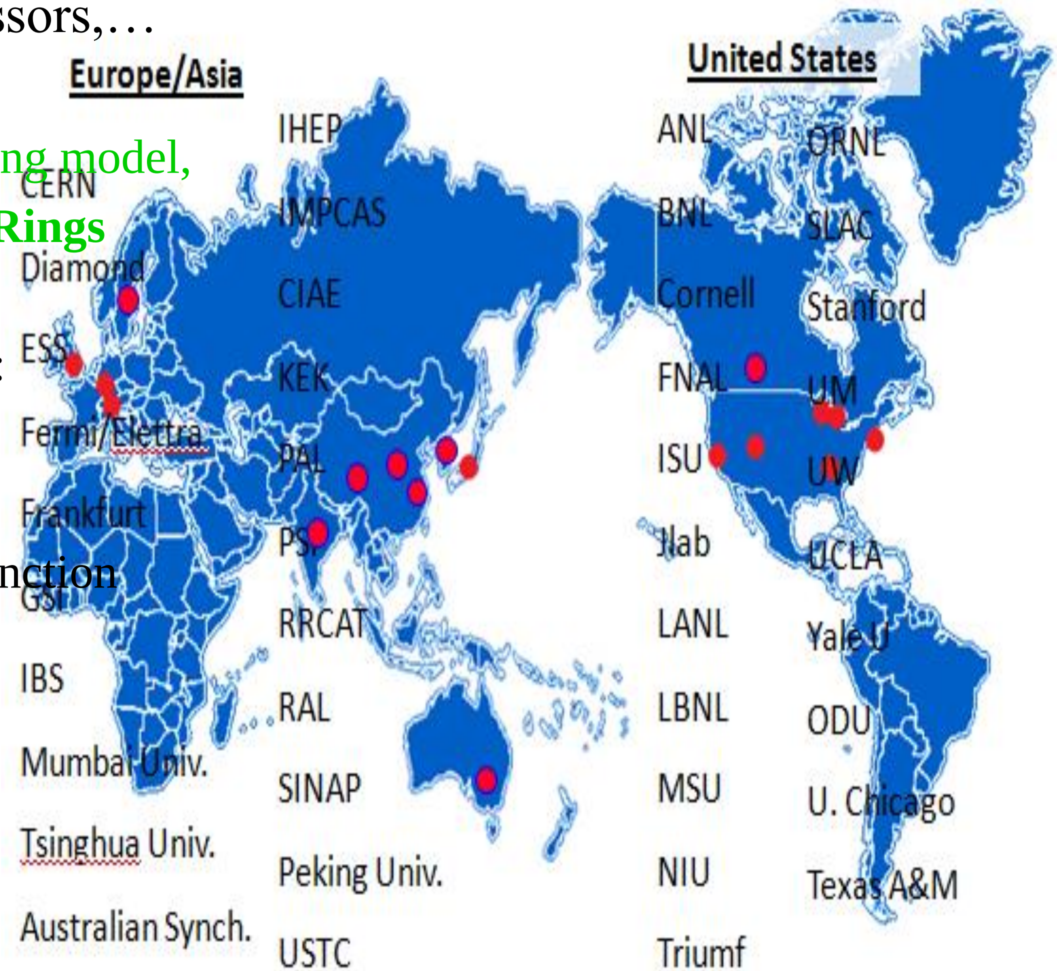
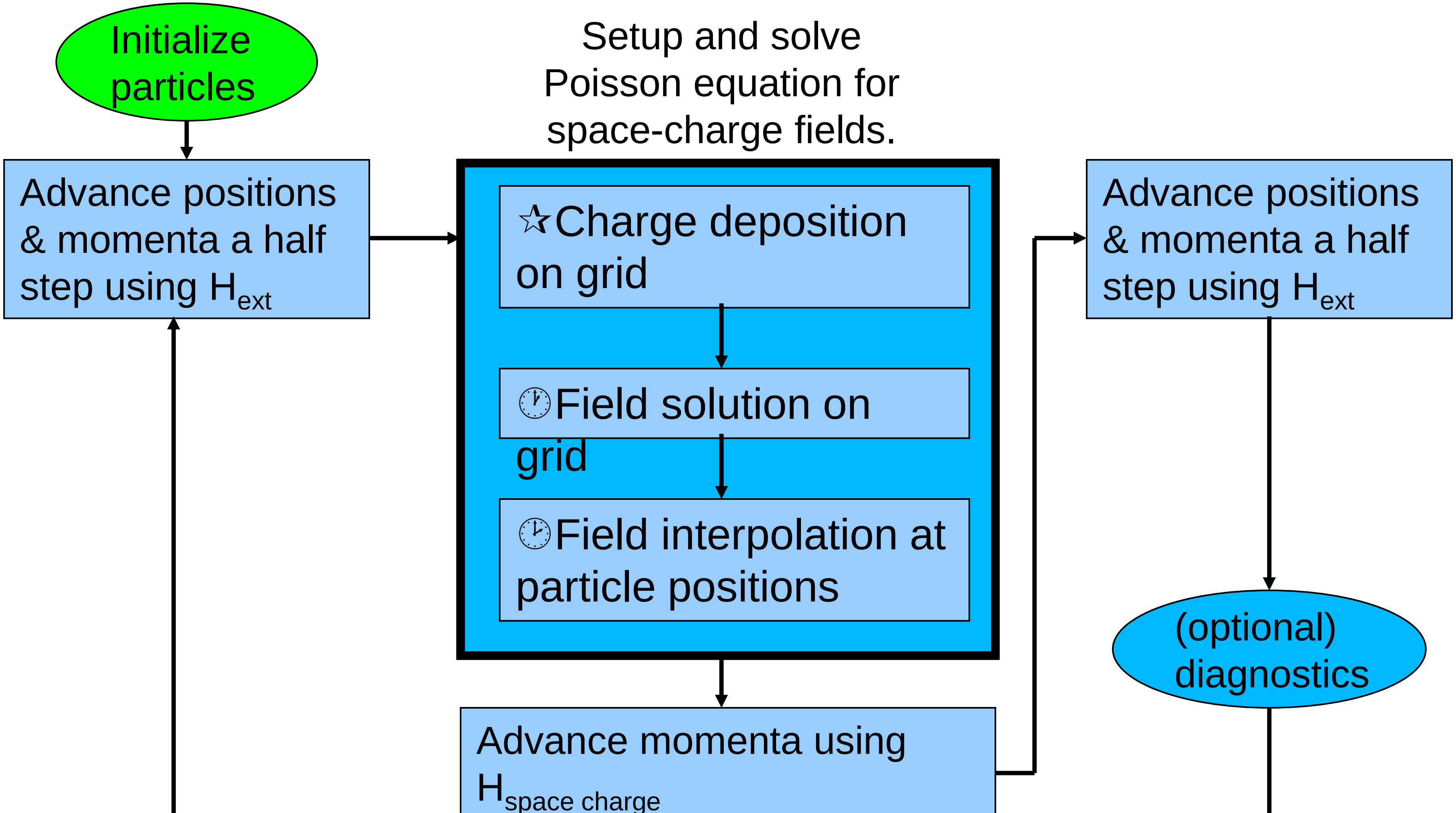
IMPACT Code Suite:
Integrated **M**ap and **P**article **AC**celerator **T**racking

- IMPACT-Z: parallel PIC code (z-code)
- IMPACT-T: parallel PIC code (t-code)
- Envelope code, pre- and post-processors,…
- Key Features
  - — Detailed RF accelerating and focusing model, beam line elements of **Linacs** and **Rings**
  - — Multiple 3D Poisson solvers
    - Variety of boundary conditions: transverse round/rectangular, longitudinal open/periodic, …
    - 3D shifted-integrated Green Function
  - — Multi-charge states, multi-bunches
  - — Machine error studies and steering
  - — Wakefields
  - — CSR/ISR
  - — Gas ionization

IMPACT has been used by researchers at more than 30 institutes and universities



Particle-In-Cell Simulation with Split-Operator Method



- Rapidly varying s-dependence of external fields is decoupled from slowly varying space charge fields
- Leads to very efficient particle advance:
  - Do not take tiny steps to push millions - billions of particles
  - Do take tiny steps to compute maps; then push particles w/ maps

IMPACT-Z for Space-Charge Study in Ring
(fully 6D symplectic tracking)

Drift – exact solution
Combined function bend – direct symplectic integrator
Quadrupole – direct symplectic integrator
RF cavity – thin lens kick
Nonlinear Multipoles – thin lens kick
Space-charge forces– lumped thin lens kick

An Example: Symlectic Tracking through a Combined Function Bend

$$H = H_1 + H_2$$

$$H_1 = -\left(1 + \frac{x}{\rho_c}\right)\sqrt{(1+\delta)^2 - p_x^2 - p_y^2} + b_0 x + b_0 \frac{x^2}{2\rho_c}$$

$$H_2 = V(x, y, \rho_c)$$

Exact solution for H_1

$$x^f = \frac{\rho_c}{b_0}\left(\frac{1}{\rho_c}\sqrt{(1+\delta)^2 - p_x^{f2} - p_y^2} - \frac{dp_x^f}{ds} - b_0\right)$$

$$p_x^f = p_x \cos\left(\frac{s}{\rho_c}\right) + \left(\sqrt{(1+\delta)^2 - p_x^2 - p_y^2} - b_0(\rho_c + x)\right) \sin\left(\frac{s}{\rho_c}\right)$$

$$y^f = y + \frac{p_y s}{b_0 \rho_c} + \frac{p_y}{b_0}\left\{\arcsin\left(\frac{p_x}{\sqrt{(1+\delta)^2 - p_y^2}}\right) - \arcsin\left(\frac{p_x^f}{\sqrt{(1+\delta)^2 - p_y^2}}\right)\right\}$$

$$p_y^f = p_y$$

$$\delta^f = \delta$$

$$\tau^f = \tau + \frac{(1+\delta)s}{b_0\rho_c} + \frac{(1+\delta)}{b_0}\left\{\arcsin\left(\frac{p_x}{\sqrt{(1+\delta)^2 - p_y^2}}\right) - \arcsin\left(\frac{p_x^f}{\sqrt{(1+\delta)^2 - p_y^2}}\right)\right\}$$

Transfer map for one step: $M(\tau) = M_2(\tau/2)M_1(\tau)M_2(\tau/2) + O(\tau^3)$

Ref: E. Forest, Beam Dynamics: A New Attitude and Framework, 1998.

Different Boundary/Beam Conditions Need Different Efficient Numerical Algorithms O(Nlog(N)) or O(N)

FFT based Green function method:

- Standard Green function: low aspect ratio beam
- Shifted Green function: separated particle and field domain
- Integrated Green function: large aspect ratio beam
- Non-uniform grid Green function: 2D radial non-uniform beam

Fully open boundary conditions

Spectral-finite difference method:

Partially open boundary
Transverse regular pipe with
longitudinal open

Multigrid spectral-finite difference method:

Transverse irregular pipe

J. Qiang, S. Paret, “Poisson solvers for self-consistent multiparticle simulations,” ICFA Mini-Workshop on Beam-Beam Effects in Hadron Colliders, March 18-22, 2013.

Green Function Solution of Poisson's Equation (I) (open boundary conditions)

$$\phi(r) = \int G(r,r')\rho(r')dr' \quad ; \; r = (x, y, z)$$

$$\phi(r_i) = h \sum_{i'=1}^{N} G(r_i - r_{i'})\rho(r_{i'})$$

$$\boxed{G(x,y,z) = 1/\sqrt{(x^2 + y^2 + z^2)}}$$

Direct summation of the convolution scales as N^2 !!!!

N – total number of grid points

FFT based Hockney's Algorithm /zero padding:- scales as (2N)log(2N)

- Ref: Hockney and Easwood, ***Computer Simulation using Particles***, McGraw-Hill Book Company, New York, 1985.

$$\phi_c(r_i) = h \sum_{i'=1}^{2N} G_c(r_i - r_{i'})\rho_c(r_{i'})$$

$$\phi(r_i) = \phi_c(r_i) \quad \text{for } i = 1, N$$

This is NOT a spectral solver!

Integrated Green Function Method (II)

(large aspect ratio beam with open boundary conditions)

$$\phi_c(r_i) = \sum_{i'=1}^{2N} G_i(r_i - r_{i'})\,\rho_c(r_{i'})$$

$$G_i(r, r') = \int G_s(r, r')\, dr'$$

integrated Green function

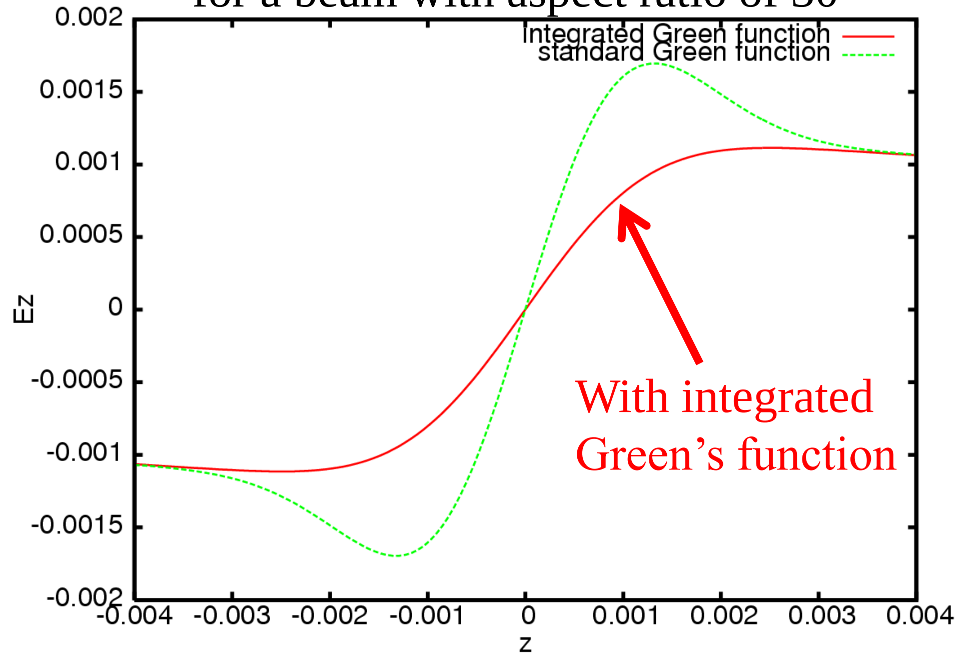
$$G_s(x, y, z) = 1/\sqrt{(x^2 + y^2 + z^2)}$$

standard Green function

Integrated Green's function is needed for modeling large aspect ratio beams!

(O(N log N))

Comparison between the IG and SG for a beam with aspect ratio of 30



R. D. Ryne, ICFA Beam DynamicsMini Workshop on Space Charge Simulation, Trinity College, Oxford, 2003

J. Qiang, S. Lidia, R. D. Ryne, and C. Limborg-Deprey, Phys. Rev. ST Accel. Beams, vol 9, 044204 (2006).

3D Poisson Solver with Transverse Rectangular Pipe (I)
(Spectral-Finite Difference Method)

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}=-\frac{\rho}{\epsilon_0}$$

with boundary conditions

$$\begin{aligned}\phi(x=0,y,z)&=0,\\ \phi(x=a,y,z)&=0,\\ \phi(x,y=0,z)&=0,\\ \phi(x,y=b,z)&=0,\\ \phi(x,y,z=\pm\infty)&=0,\end{aligned}$$

$$\rho(x,y,z)=\sum_{l=1}^{N_l}\sum_{m=1}^{N_m}\rho^{lm}(z)\sin(\alpha_l x)\sin(\beta_m y),$$

$$\phi(x,y,z)=\sum_{l=1}^{N_l}\sum_{m=1}^{N_m}\phi^{lm}(z)\sin(\alpha_l x)\sin(\beta_m y),$$

where

$$\rho^{lm}(z)=\frac{4}{ab}\int_0^a\int_0^b\rho(x,y,z)\sin(\alpha_l x)\sin(\beta_m y),$$

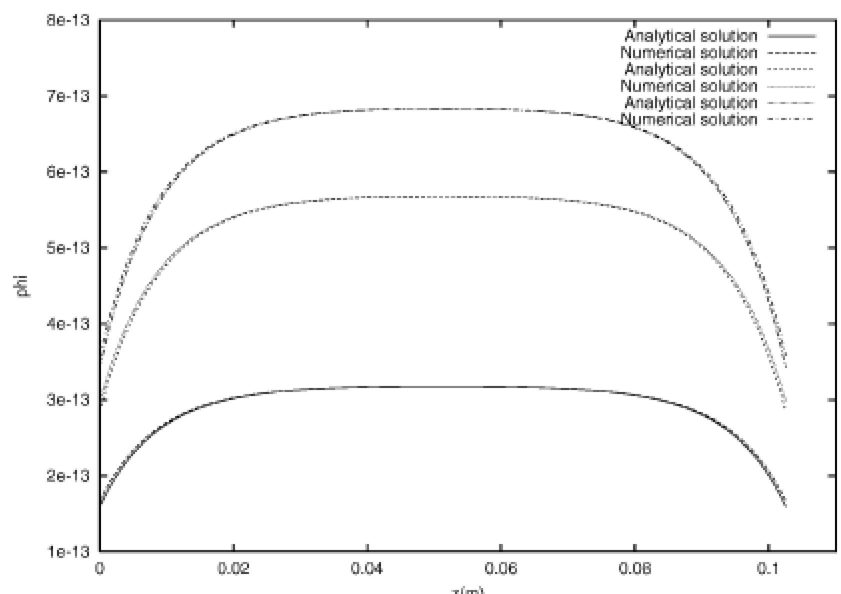
$$\phi^{lm}(z)=\frac{4}{ab}\int_0^a\int_0^b\phi(x,y,z)\sin(\alpha_l x)\sin(\beta_m y),$$

$$\frac{\partial^2\phi^{lm}(z)}{\partial z^2}-\gamma_{lm}^2\phi^{lm}(z)=-\frac{\rho^{lm}(z)}{\epsilon_0},$$

$$\frac{\phi^{lm}_{n+1}-2\phi^{lm}_n+\phi^{lm}_{n-1}}{h_z^2}-\gamma_{lm}^2\phi^{lm}_n=-\frac{\rho^{lm}_n}{\epsilon_0},$$

$$\begin{aligned}\phi^{lm}_{-1}&=\exp(-\gamma_{lm}h_z)\phi^{lm}_0, && n=0,\\ \phi^{lm}_{N+1}&=\exp(-\gamma_{lm}h_z)\phi^{lm}_N, && n=N.\end{aligned}$$

Numerical Solutions vs. Analytical Solutions



z (m)

J. Qiang, and R. Ryne, Comput. Phys. Comm. 138, p. 18 (2001).

3D Poisson Solver with Transverse Rectangular Pipe (II)
(Spectral-Green Function Method and 3D Spectral Method)

$$\frac{\partial^2 \phi^{lm}(z)}{\partial z^2} - \gamma_{lm}^2 \phi^{lm}(z) = -\frac{\rho^{lm}(z)}{\epsilon_0},$$

Green function method:
- efficiently handle long bunch

$$\phi^{lm}(z) = \frac{-1}{2\gamma_{lm}\varepsilon_0}\int \exp(-\gamma_{lm}|z-z'|)\rho^{lm}(z')dz'$$

$$\phi^{lm}(z) = \frac{-1}{2\gamma_{lm}\varepsilon_0}\sum_j \rho^{lm}(z_j')G(z-z_j')$$

$$G(z-z') = \int_{z'-h/2}^{z'+h/2} \exp(-\gamma_{lm}|z-t|)dt$$

spectral method:
-reduce numerical noise with filtering in frequency domain

$$\phi^{lm}(z) = \sum_n \phi_n^{lm} H_n(z); \; \rho^{lm}(z) = \sum_n \rho_n^{lm} H_n(z)$$

Hermite polynomial H_n: $\int_{-\infty}^{\infty} H_n(z) H_m(z) dz = 2^n n! \sqrt{\pi}\delta_{mn}$

$$\frac{1}{4}\phi_{n-2}^{lm} - (\frac{1}{2}(2n+1) + \gamma_{lm}^2)\phi_n^{lm} + (n+2)(n+1)\phi_{n+2}^{lm} = A^2 \rho_n^{lm}$$

J. Qiang, in progress (2014).

3D Poisson Solver with Transverse Rectangular Pipe (III)
(Green Function Method)

$$G(x,x',y,y',z,z') = \frac{1}{2\pi ab}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{1}{\kappa_{mn}}\sin\frac{m\pi x}{a}\sin\frac{m\pi x'}{a}\sin\frac{n\pi y}{b}\sin\frac{n\pi y'}{b}e^{-\kappa_{mn}|z-z'|},$$

$$\begin{aligned} G \;=\; & R(x-x',y-y',z-z') - R(x-x',y+y',z-z') \\ & -R(x+x',y-y',z-z') + R(x+x',y+y',z-z'), \end{aligned}$$

$$R(u,v,w) = \frac{1}{2\pi ab}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{1}{\kappa_{mn}}\cos\frac{m\pi u}{a}\cos\frac{n\pi v}{b}e^{-\kappa_{mn}|w|}.$$

$$\begin{aligned} & \phi_{i,j,k}/(h_x h_y h_z) = \\ & \mathcal{F}^{bbb}\{(\mathcal{F}^{fff}\rho_{i,j,k})(\mathcal{F}^{fff}R_{i,j,k})\} - \mathcal{F}^{bfb}\{(\mathcal{F}^{fff}\rho_{i,j,k})(\mathcal{F}^{fbf}R_{i,j,k})\} \\ & -\mathcal{F}^{fbb}\{(\mathcal{F}^{fff}\rho_{i,j,k})(\mathcal{F}^{bff}R_{i,j,k})\} + \mathcal{F}^{ffb}\{(\mathcal{F}^{fff}\rho_{i,j,k})(\mathcal{F}^{bbf}R_{i,j,k})\} \end{aligned}$$

$$g_z = \frac{1}{h_z^2}\int_{z_k}^{z_{k+1}} dz'\left[\rho_k(h_z-(z'-z_k)) + \rho_{k+1}\,(z'-z_k)\right]e^{-\kappa_{mn}|z-z'|}.$$

$$R_{int}(u,v,w) = \frac{1}{2\pi ab}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{1}{\kappa_{mn}}\cos\frac{m\pi u}{a}\cos\frac{n\pi v}{b}g_z(w).$$

$$g_z(w) = \frac{1}{h_z^2\kappa_{mn}^2}\left[2h_z\kappa_{mn}\delta_{w,0} + \left(e^{-\kappa_{mn}|w+h_z|} - 2e^{-\kappa_{mn}|w|} + e^{-\kappa_{mn}|w-h_z|}\right)\right],$$

Pro: computational domain needs to contain only the beam itself.

Con: more numerical operations for Green function evaluation.

R. Ryne, arXiv :1111, 4971, 2011.

SIS-18 Benchmark

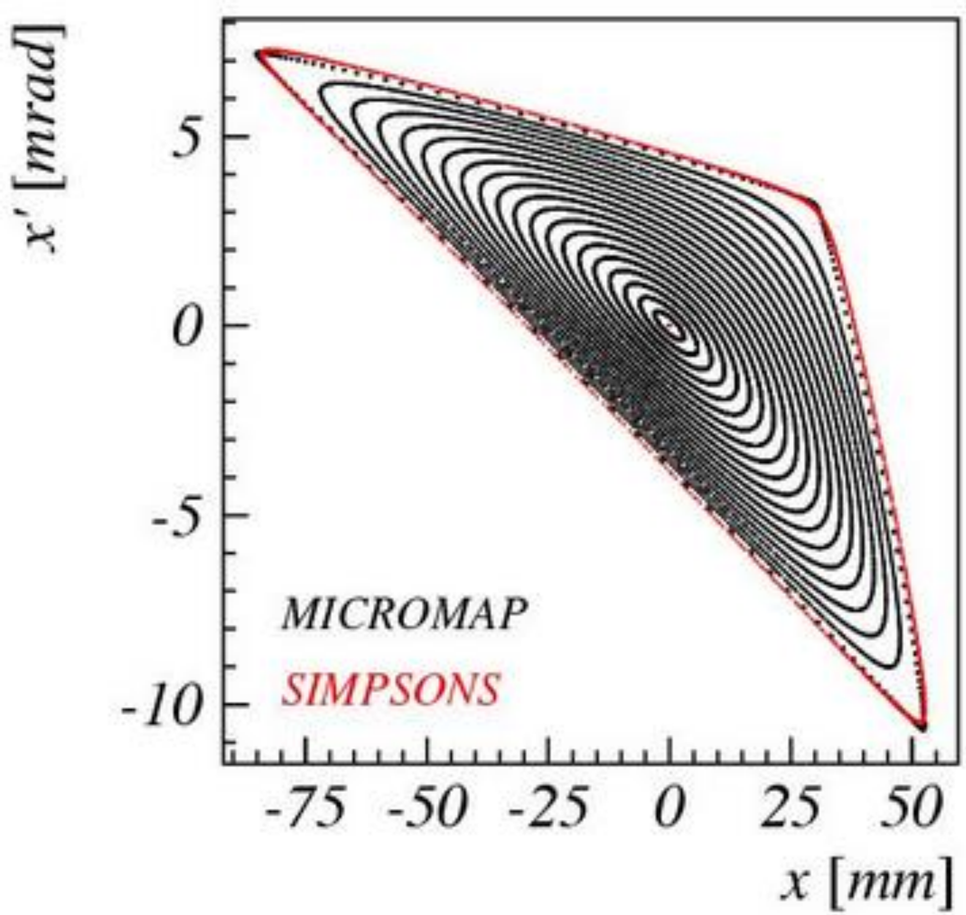
PARAMETERS for setps 1-6

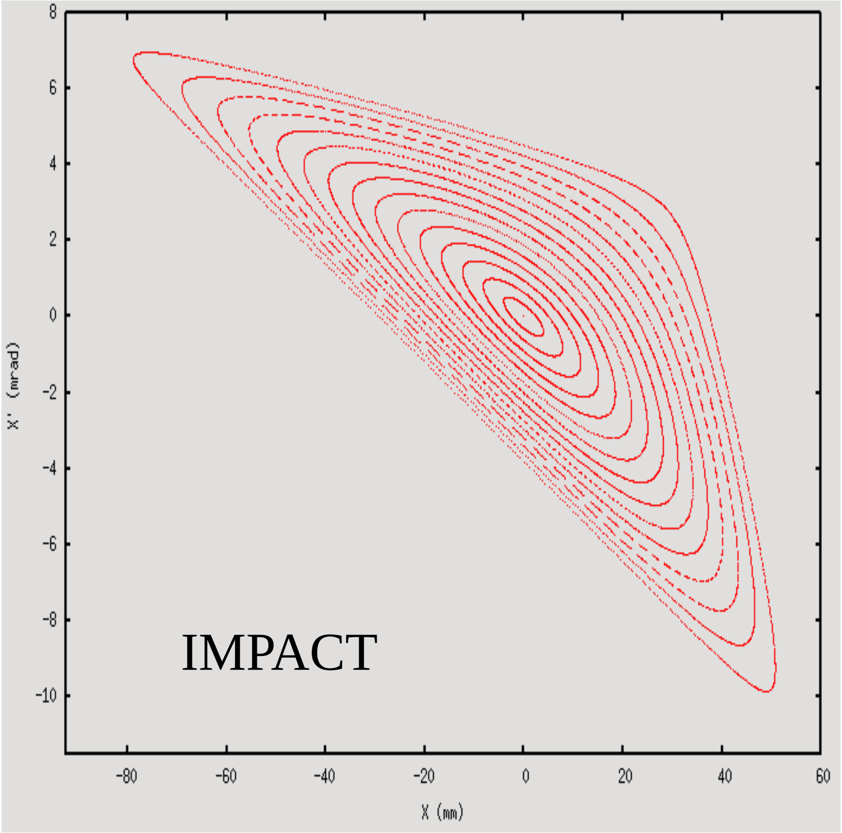
Lattice SIS18	
Strength of the sextupole (when used)	$K_2 = 0.2\ m^{-2}$
Maximum tuneshift	$\Delta Q_x = 0.1$
Horizontal transverse size (rms)	$X_{rms} = 5$ mm
Vertical transverse size (rms)	$Y_{rms} = 5$ mm
Longitudinal size (rms)	$Z_{rms} = 40.35$ m
Horizontal emittance (2 σ)	$\varepsilon_x = 12.57$ mm mrad
Vertical emittance (2 σ)	$\varepsilon_y = 9.30$ mm mrad
Turns for 1 synchrotron oscillation	$N_{synch} = 15000$
Bunch length (4 σ_z)	$\tau = 3472.7$ ns
Kinetik energy	$E_k = 11.4$ MeV/u
Gamma transition	$\gamma_t = 5$
momentum spread at $3\sigma_z$	$\Delta p/p = 2.5 \times 10^{-4}$

http://web-docs.gsi.de/~giuliano/

Benchmark Step 1: Single Particle Phase Space

Qx = 4.338, Qy = 3.2





All three codes show very close phase space topology.

PARAMETERS for setps 7-8

Lattice SIS18	
Strength of the sextupole (when used)	$K_2 = 0.2\ m^{-2}$
Maximum tuneshift	$\Delta Q_x = 0.1$
Horizontal transverse size (rms)	$X_{rms} = 5$ mm
Vertical transverse size (rms)	$Y_{rms} = 5$ mm
Longitudinal size (rms)	$Z_{rms} = 2.69$ m
Horizontal emittance (2 σ)	$\varepsilon_x = 12.57$ mm mrad
Vertical emittance (2 σ)	$\varepsilon_y = 9.30$ mm mrad
Turns for 1 synchrotron oscillation	$N_{synch} = 1000$
Bunch length (4 σ_z)	$\tau = 231.51$ ns
Kinetik energy	$E_k = 11.4$ MeV/u
Gamma transition	$\gamma_t = 5$
momentum spread at $3\sigma_z$	$\Delta p/p = 2.5 \times 10^{-4}$

Parameters for step 9:

- Qx = 4.3604, Qy = 3.2
- RF cavity voltage: 152 V
- RF frequency: 0.214456 MHz
- X aperture : 40 cm
- Y aperture: 30 cm

Generate Initial Matched Beam Distribution
(Normal Form Transformation)

For a given particle phase space coordinate: $\xi = (x, p_x, y, p_y, z, p_z)^T$

after one turn through the ring $\xi^{n+1} = M\xi^n$ where M is the one-turn transfer matrix

Define a second order moments matrix of the distribution:

$$\Sigma = \begin{pmatrix} \langle xx\rangle & \langle xp_x\rangle & \langle xy\rangle & \langle xp_y\rangle & \langle xz\rangle & \langle xp_z\rangle \\ \langle p_x x\rangle & \langle p_x p_x\rangle & \langle p_x y\rangle & \langle p_x p_y\rangle & \langle p_x z\rangle & \langle p_x p_z\rangle \\ \langle yx\rangle & \langle yp_x\rangle & \langle yy\rangle & \langle yp_y\rangle & \langle yz\rangle & \langle yp_z\rangle \\ \langle p_y x\rangle & \langle p_y p_x\rangle & \langle p_y y\rangle & \langle p_y p_y\rangle & \langle p_y z\rangle & \langle p_y p_z\rangle \\ \langle zx\rangle & \langle zp_x\rangle & \langle zy\rangle & \langle zp_y\rangle & \langle zz\rangle & \langle zp_z\rangle \\ \langle p_z x\rangle & \langle p_z p_x\rangle & \langle p_z y\rangle & \langle p_z p_y\rangle & \langle p_z z\rangle & \langle p_z p_z\rangle \end{pmatrix},$$

after one turn: $\Sigma^{n+1} = M\Sigma^n M^T$

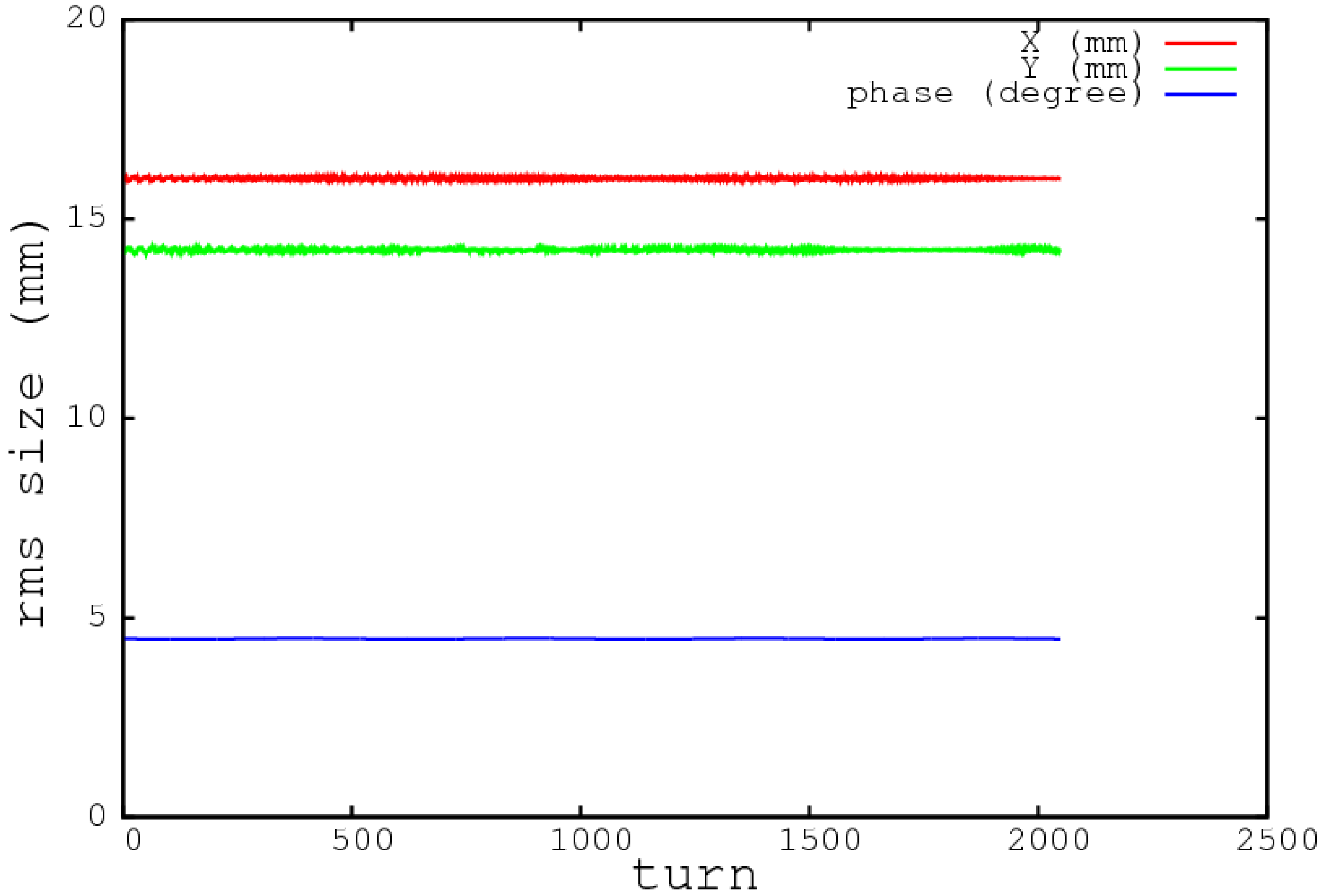
For an envelope matched beam: $\Sigma^n = M\Sigma^n M^T$

Let: $M = ANA^{-1}$ where N is the normal form matrix

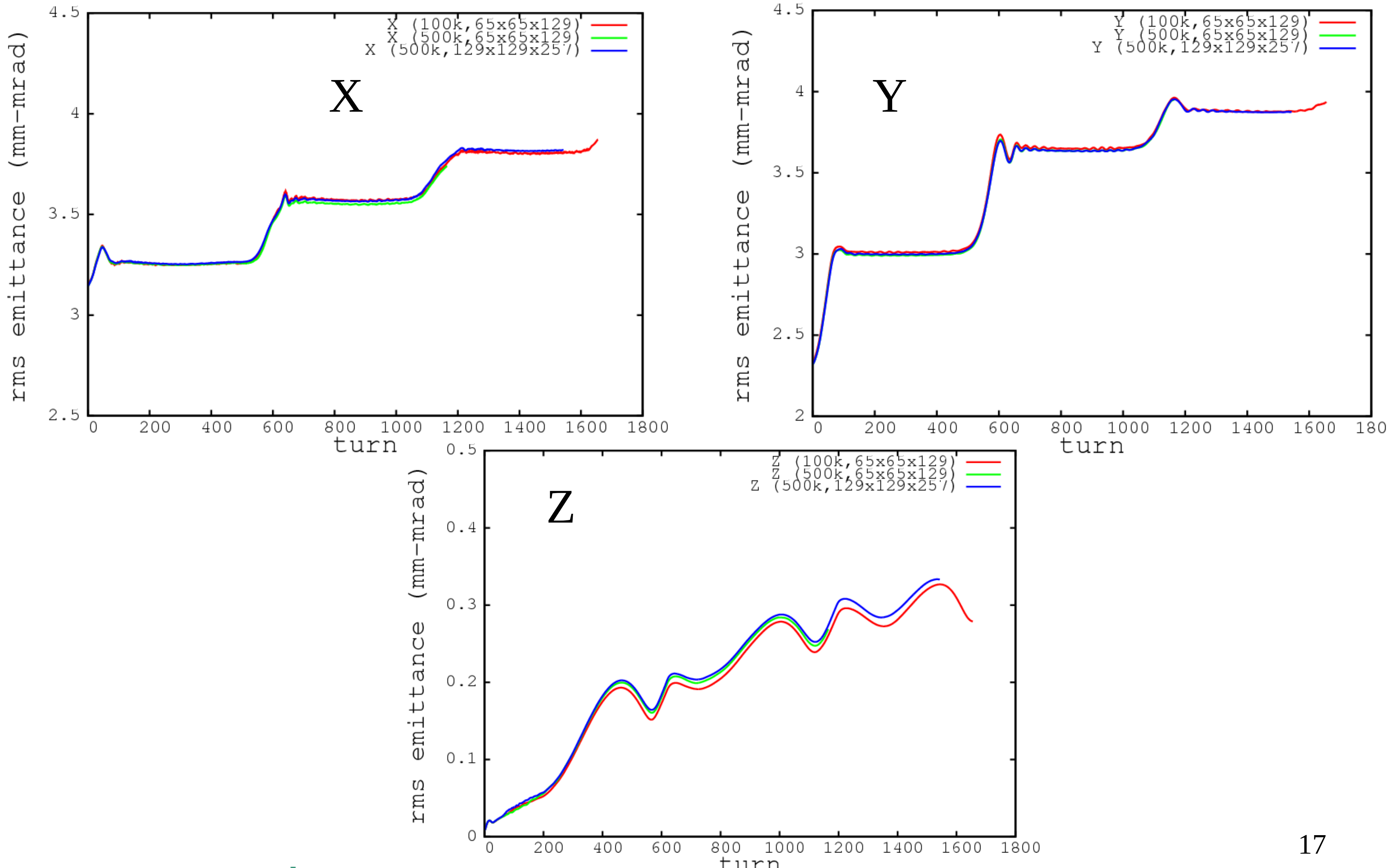
$$(A^{-1}\Sigma^n A^{-T}) = N(A^{-1}\Sigma^n A^{-T})N^T$$

For the given emittances in the phase space coordinate, one can find the corresponding emittances in the normal coordinates to generate a matched beam distribution.

Evolution of RMS Beam Sizes with the Initial Matched Distribution (no space-charge)

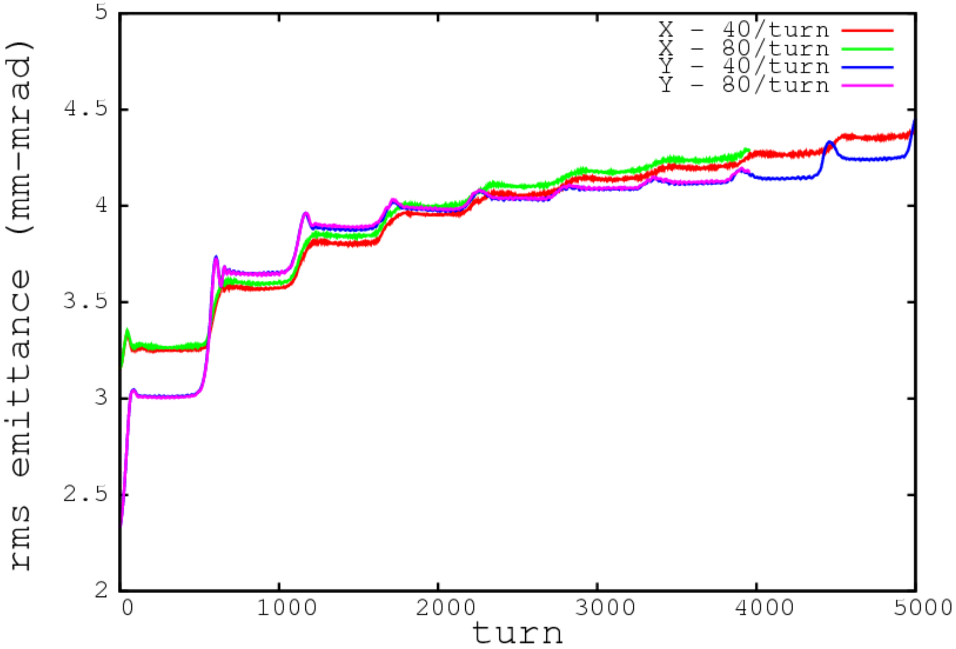


Numerical Test of Convergence: Evolution of RMS Beam Emittances (1) (with space-charge)

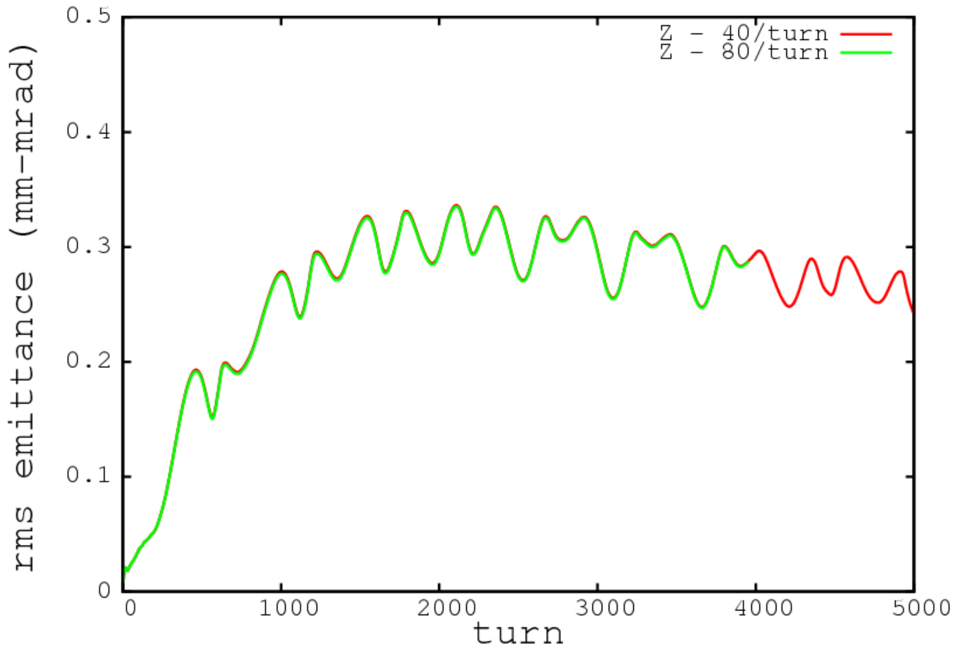


Numerical Test of Convergence: Evolution of RMS Beam Emittances (II) (with space-charge)

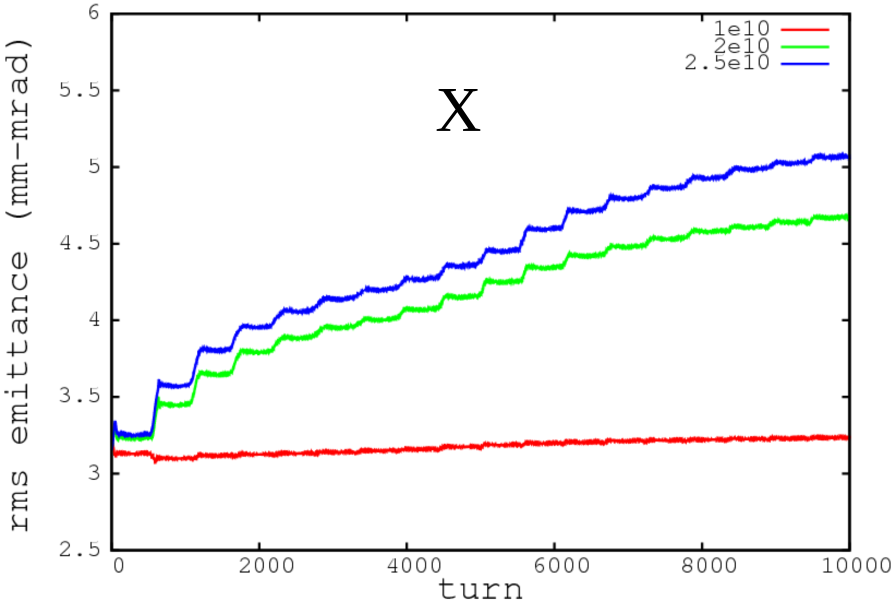
Transverse

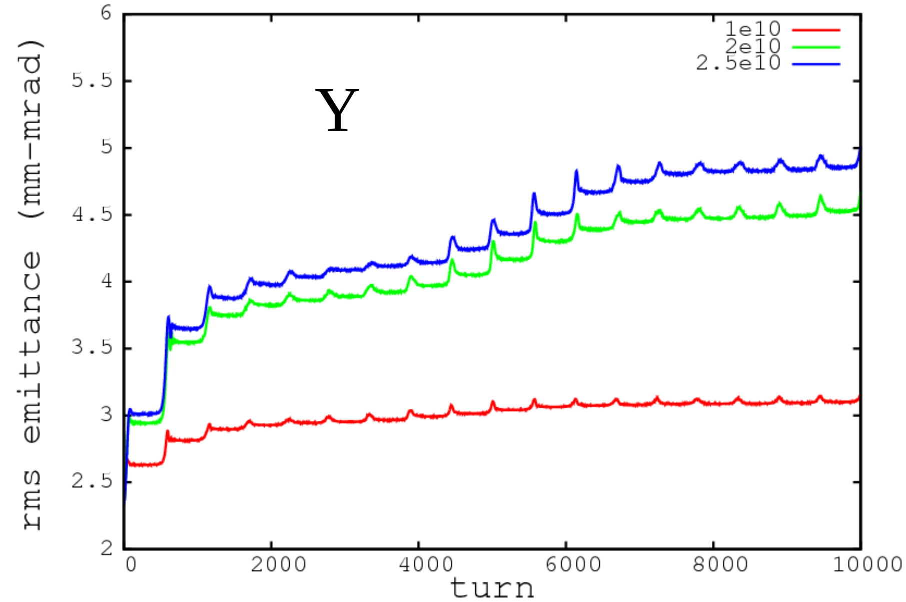


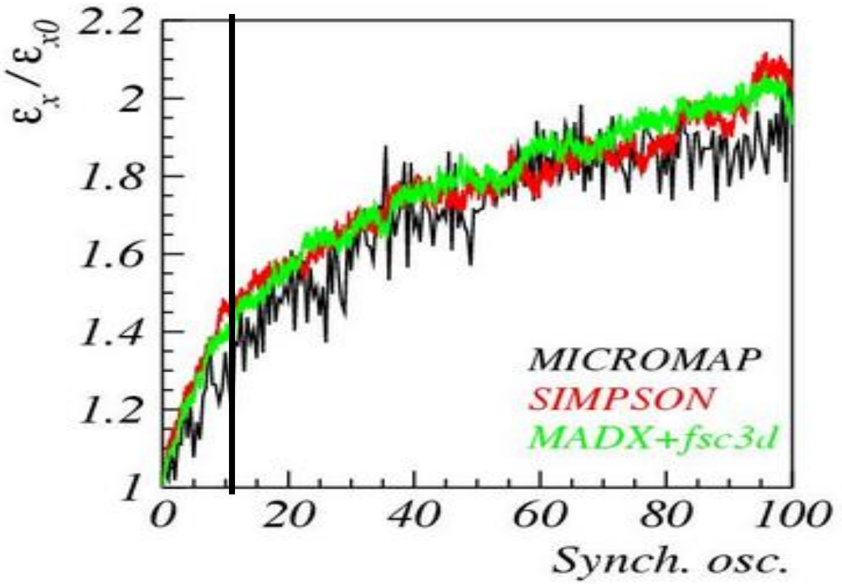
Longitudinal

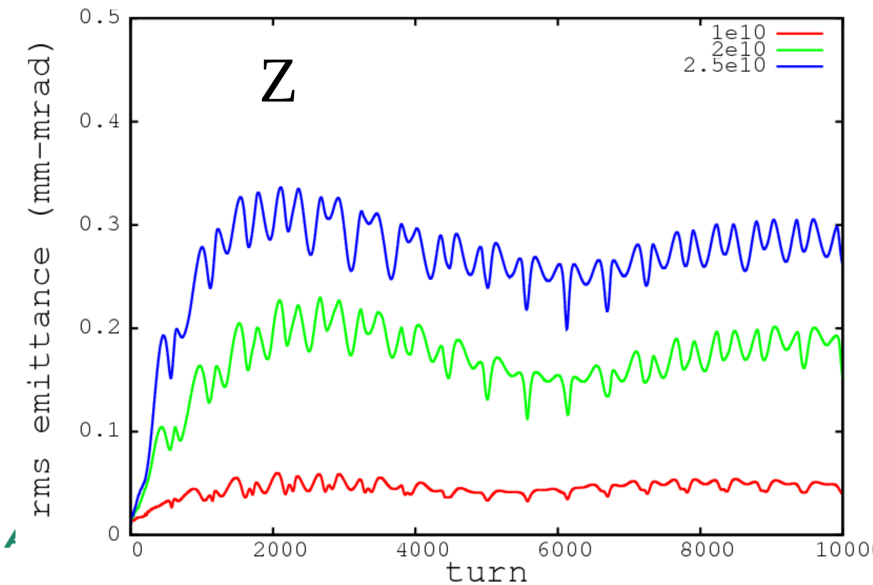


Evolution of RMS Beam Emittances: Different Beam Intensity

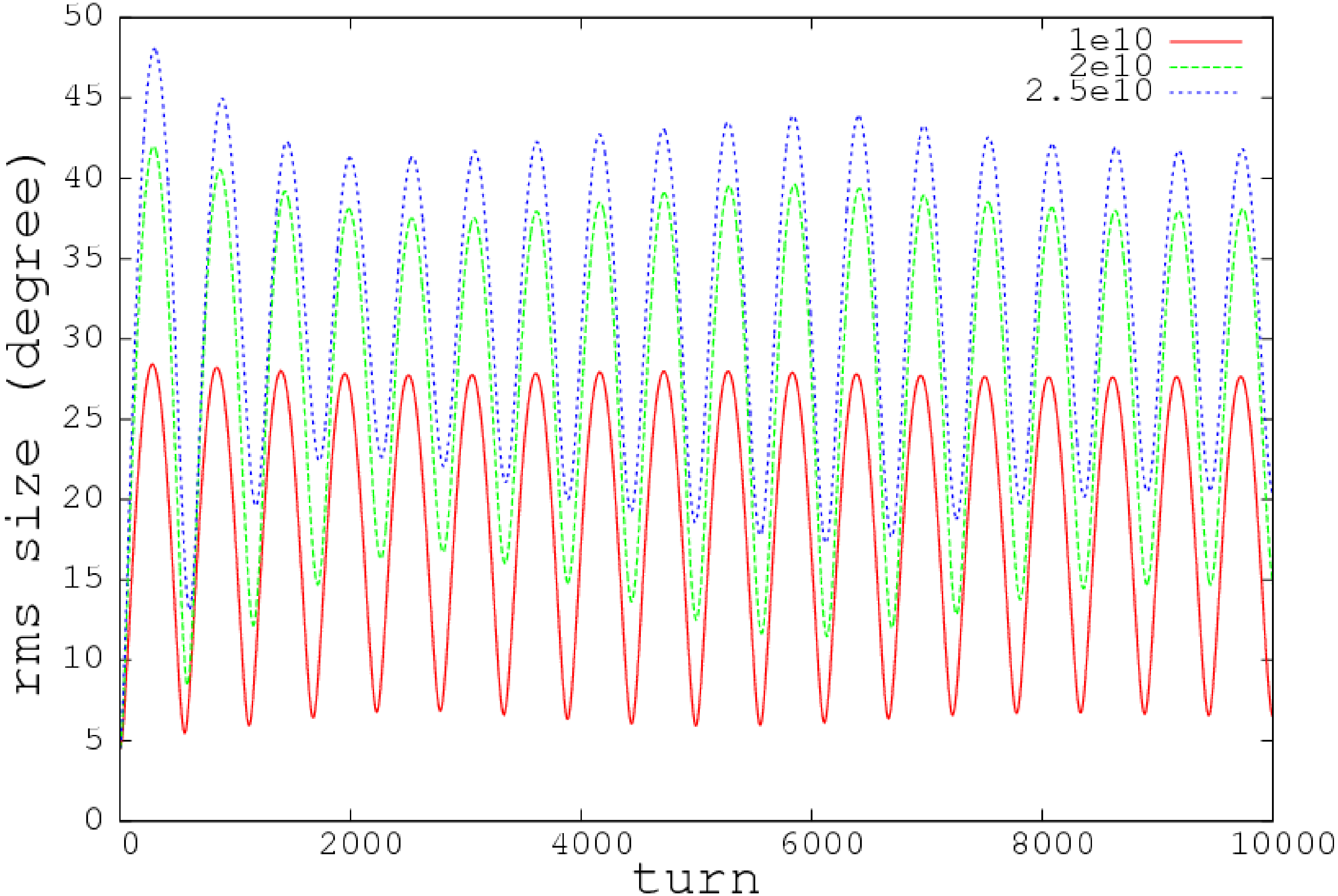








Evolution of RMS Bunch Length: Different Beam Intensity



An Application Example: PS Montague Resonace

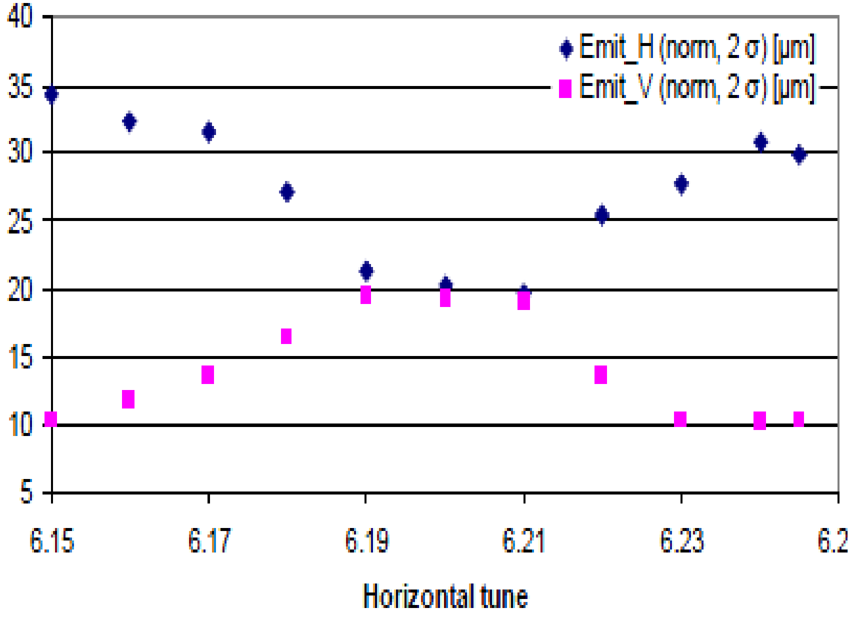
Physical parameters:

RF frequency = 3.5 MHz
RF voltage = 27 kV
Ek = 1.4 GeV
Emit_x = 7.5 mm-mrad
Emit_y = 2.5 mm-mrad
Rms bunch length = 45 ns
Rms dp/p = 1.7×10^{-3}

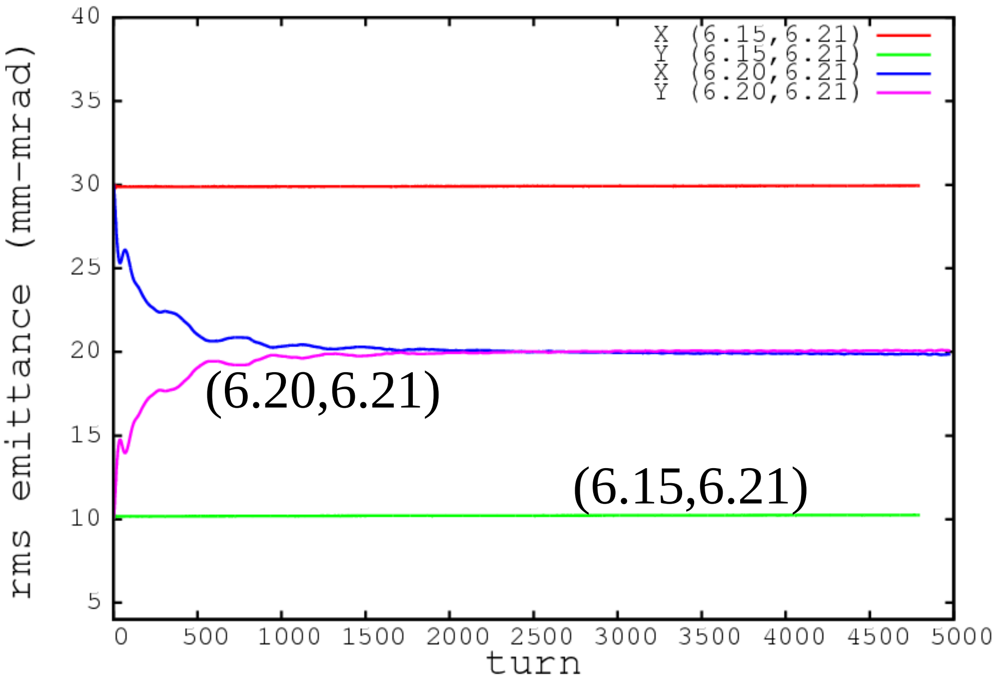
Horizontal tune: 6.15 – 6.245
Vertical tune: 6.21
Synchrotron period: 1.5 ms
Half Aperture = 7cm x 3.5cm
I = 1.0×10^{12}

Refs: B. W. Montague, CERN-Report No. 68-38, CERN, 1968.
E. Metral et al., Proc. of EPAC 2004, p. 1894.
I. Hofmann et al., Proc. of EPAC 2004, p. 1960.

measurements



Simulation



Thank You for Your Attention!